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DETERMINATION OF LIGANDS FOR PROTEINS Frommel et al.

Appl. No.: 09/772,538 Atty Docket: ABOHM1.001CP1

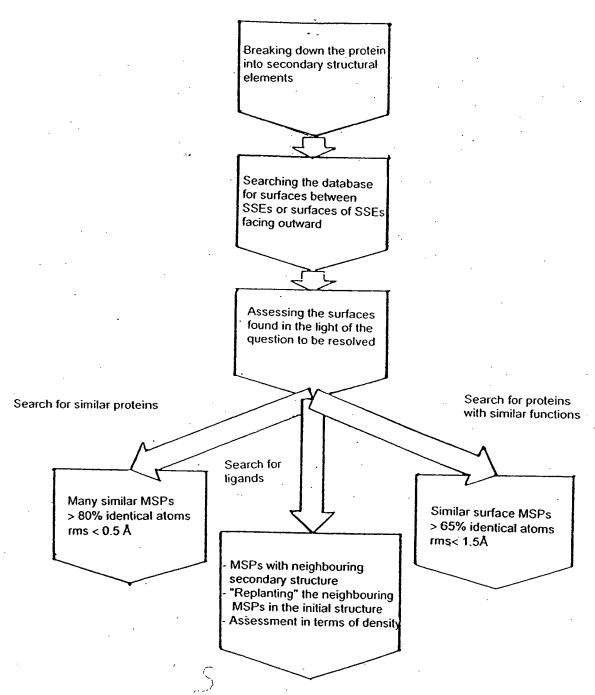


Figure 1

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The Principle of Ligand Identification Dictionary of Interfaces The Process in Proteins Goal: Identification of a ligand that binds to a predefined protein surface area (active site) Dissection of the protein surface in molecular surface patches (MSPs) Definition of MSP(s) forming the active site for which a ligand has to be identified Search for MSPs (basis patches) in the databank that are similar to the active site MSP(s) with respect to geometric parameters SSE with basis patch and fitting atomic species SSE with contact patch The contact patch is supposed to be complementary to the active site MSP. Transformation of co-ordinates of the contact patch-SSEs on the active site MSP evaluation of the fit by local atomic density [3]. The "Dictionary of Interfaces in Proteins" (DIP) is a collection of interfaces that are defined as pairs of matching molecular surface patches between neighboring secondary structural elements. Each interface consists of two subsets of atoms from Abbreviations: neighbouring secondary structure elements (pairs of SSE: secondary structual element complemetary MSPs). All such interfaces from known protein

structures were collected in a comprehensive data bank (DIP).

MSP: molecular surface patch